wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 21, 2023 – 04:11 PM JST

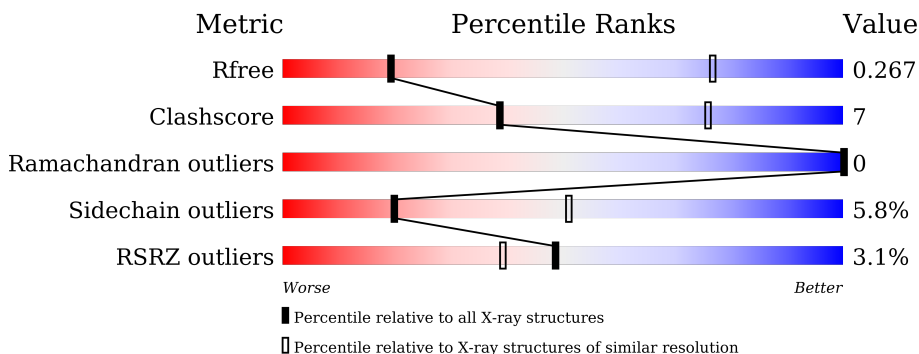|		
PDB ID	:	7VW7
Title	:	Crystal structure of the 2 ADP-AlF4-bound V1 complex
Authors	:	Suzuki, K.; Shekhar, M.; Gupta, C.; Singharoy, A.; Murata, T.
Deposited on	:	2021-11-09
Resolution	:	3.82 Å(reported)

1   Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.82 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Rfree		0.267
Clashscore		7
Ramachandran outliers		0
Sidechain outliers		5.8%
RSRZ outliers		3.1%

Worse   Better

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1231 (4.04-3.60)
Clashscore	141614	1031 (4.02-3.62)
Ramachandran outliers	138981	1261 (4.04-3.60)
Sidechain outliers	138945	1255 (4.04-3.60)
RSRZ outliers	127900	1139 (4.04-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	600	3% / 79% / 17% / · ·
1	B	600	3% / 83% / 15% / ··
1	C	600	4% / 80% / 15% / · ·
2	D	465	81% / 15% / · ·
2	E	465	2% / 80% / 16% / · ·
2	F	465	2% / 73% / 22% / · ·

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Mol	Chain	Length	Quality of chain
3	G	217	5% · · · 59% · · 14% · 24%
4	H	115	10% · · 80% · · 14%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	ALF	B	603	-	-	X	-

2 Entity composition ⓘ

There are 9 unique types of molecules in this entry. The entry contains 25072 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called V-type sodium ATPase catalytic subunit A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	588	Total	C	N	O	S	Se	0	0	0
			4320	2718	724	852	3	23			
1	B	593	Total	C	N	O	S	Se	0	0	0
			4370	2732	740	872	3	23			
1	C	579	Total	C	N	O	S	Se	0	0	0
			4220	2604	729	861	3	23			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	expression tag	UNP A0A1V8WY35
A	-5	SER	-	expression tag	UNP A0A1V8WY35
A	-4	SER	-	expression tag	UNP A0A1V8WY35
A	-3	GLY	-	expression tag	UNP A0A1V8WY35
A	-2	SER	-	expression tag	UNP A0A1V8WY35
A	-1	SER	-	expression tag	UNP A0A1V8WY35
A	0	GLY	-	expression tag	UNP A0A1V8WY35
B	-6	GLY	-	expression tag	UNP A0A1V8WY35
B	-5	SER	-	expression tag	UNP A0A1V8WY35
B	-4	SER	-	expression tag	UNP A0A1V8WY35
B	-3	GLY	-	expression tag	UNP A0A1V8WY35
B	-2	SER	-	expression tag	UNP A0A1V8WY35
B	-1	SER	-	expression tag	UNP A0A1V8WY35
B	0	GLY	-	expression tag	UNP A0A1V8WY35
C	-6	GLY	-	expression tag	UNP A0A1V8WY35
C	-5	SER	-	expression tag	UNP A0A1V8WY35
C	-4	SER	-	expression tag	UNP A0A1V8WY35
C	-3	GLY	-	expression tag	UNP A0A1V8WY35
C	-2	SER	-	expression tag	UNP A0A1V8WY35
C	-1	SER	-	expression tag	UNP A0A1V8WY35
C	0	GLY	-	expression tag	UNP A0A1V8WY35

- Molecule 2 is a protein called V-type sodium ATPase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	452	Total 3375	C 2121	N 587	O 653	Se 14	0	0	0
2	E	452	Total 3423	C 2153	N 587	O 669	Se 14	0	0	0
2	F	453	Total 3445	C 2181	N 589	O 661	Se 14	0	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	GLY	-	expression tag	UNP A0A1V8XC32
D	-5	SER	-	expression tag	UNP A0A1V8XC32
D	-4	SER	-	expression tag	UNP A0A1V8XC32
D	-3	GLY	-	expression tag	UNP A0A1V8XC32
D	-2	SER	-	expression tag	UNP A0A1V8XC32
D	-1	SER	-	expression tag	UNP A0A1V8XC32
D	0	GLY	-	expression tag	UNP A0A1V8XC32
E	-6	GLY	-	expression tag	UNP A0A1V8XC32
E	-5	SER	-	expression tag	UNP A0A1V8XC32
E	-4	SER	-	expression tag	UNP A0A1V8XC32
E	-3	GLY	-	expression tag	UNP A0A1V8XC32
E	-2	SER	-	expression tag	UNP A0A1V8XC32
E	-1	SER	-	expression tag	UNP A0A1V8XC32
E	0	GLY	-	expression tag	UNP A0A1V8XC32
F	-6	GLY	-	expression tag	UNP A0A1V8XC32
F	-5	SER	-	expression tag	UNP A0A1V8XC32
F	-4	SER	-	expression tag	UNP A0A1V8XC32
F	-3	GLY	-	expression tag	UNP A0A1V8XC32
F	-2	SER	-	expression tag	UNP A0A1V8XC32
F	-1	SER	-	expression tag	UNP A0A1V8XC32
F	0	GLY	-	expression tag	UNP A0A1V8XC32

- Molecule 3 is a protein called V-type sodium ATPase subunit D.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	G	165	Total 1207	C 750	N 219	O 230	S 1	Se 7	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-6	GLY	-	expression tag	UNP A0A7Z9AX30
G	-5	SER	-	expression tag	UNP A0A7Z9AX30

WORLDWIDE
wwPDB
PROTEIN DATA BANK

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-4	SER	-	expression tag	UNP A0A7Z9AX30
G	-3	GLY	-	expression tag	UNP A0A7Z9AX30
G	-2	SER	-	expression tag	UNP A0A7Z9AX30
G	-1	SER	-	expression tag	UNP A0A7Z9AX30
G	0	GLY	-	expression tag	UNP A0A7Z9AX30

- Molecule 4 is a protein called V-type sodium ATPase subunit NtpG (F).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
4	H	99	639	402	107	128	1	1	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	104	SER	-	expression tag	UNP A0A1V8XC17
H	105	GLY	-	expression tag	UNP A0A1V8XC17
H	106	PRO	-	expression tag	UNP A0A1V8XC17
H	107	SER	-	expression tag	UNP A0A1V8XC17
H	108	SER	-	expression tag	UNP A0A1V8XC17
H	109	GLY	-	expression tag	UNP A0A1V8XC17
H	110	GLU	-	expression tag	UNP A0A1V8XC17
H	111	ASN	-	expression tag	UNP A0A1V8XC17
H	112	LEU	-	expression tag	UNP A0A1V8XC17
H	113	TYR	-	expression tag	UNP A0A1V8XC17
H	114	PHE	-	expression tag	UNP A0A1V8XC17
H	115	GLN	-	expression tag	UNP A0A1V8XC17

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

ADP
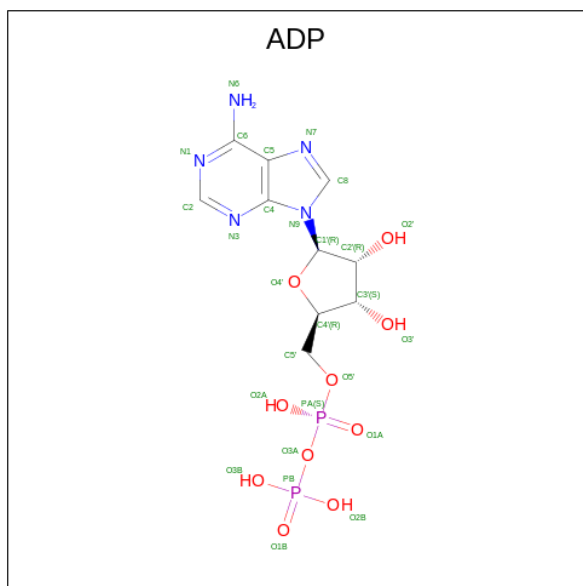
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total Mg 1 1	0	0
7	C	1	Total Mg 1 1	0	0

- Molecule 8 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula: AlF_4) (labeled as "Ligand of Interest" by depositor).
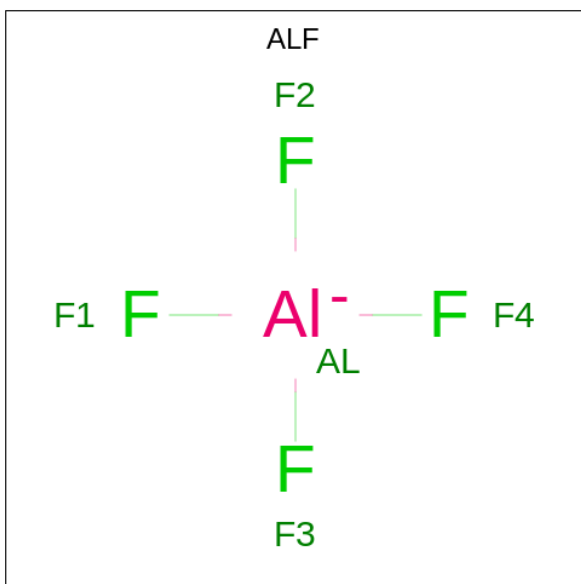
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total Al F 5 1 4	0	0
8	C	1	Total Al F 5 1 4	0	0

- Molecule 9 is water.

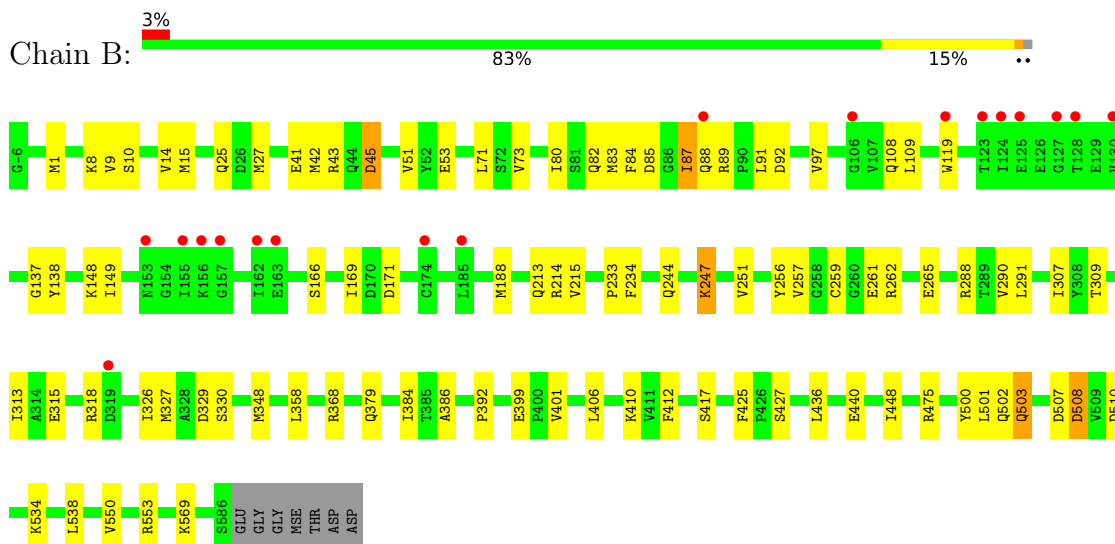| Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total O 1 1	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
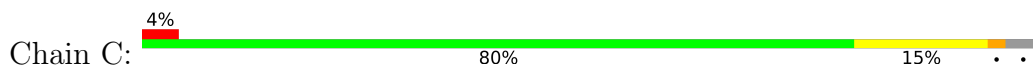
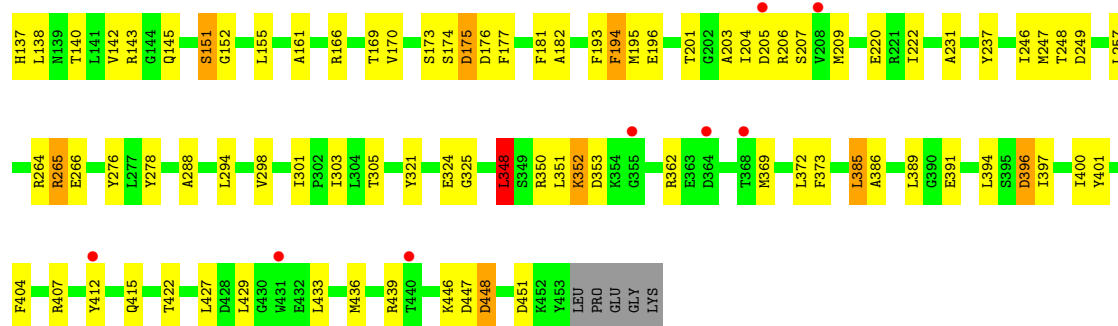• Molecule 1: V-type sodium ATPase catalytic subunit A

Chain A:

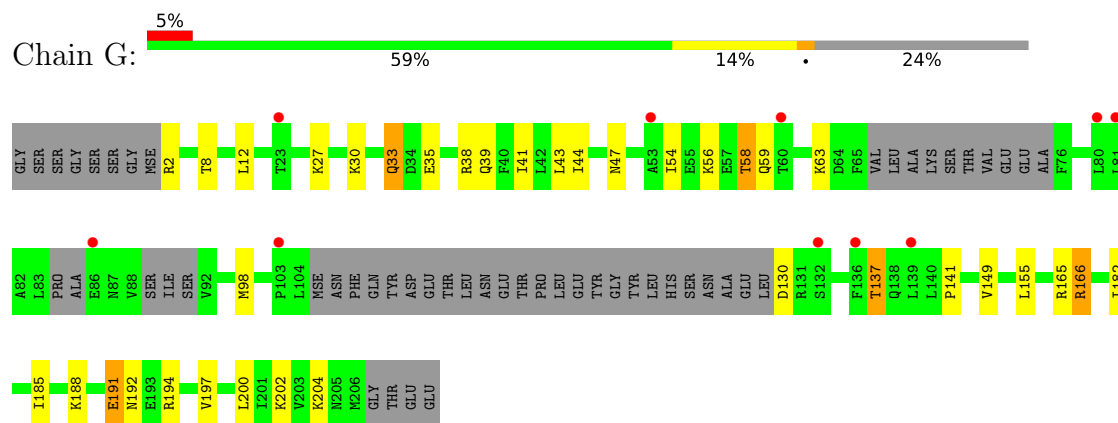• Molecule 1: V-type sodium ATPase catalytic subunit A

Chain B:
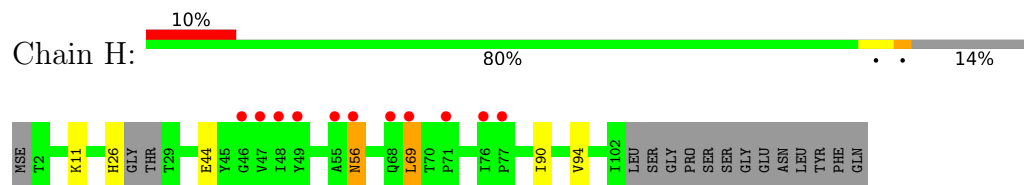
• Molecule 1: V-type sodium ATPase catalytic subunit A

Chain C:

GLY SER SER GLY SER GLY | M1 S20 I24 Q25 C28 E38 E41 M42 S48 I49 Q50 V51 Y52 E53 R65 G76 P77 S81 P90 L91 D92 F102 Q108 A111 L112 T123 G127 T128 E129 V130 I135 I136 D140 K156

Q160 F167 D171 C174 L185 Q201 P208 Q213 R214 T218 T223 P233 A236 V240 S249 R262 E265 M266 T267 M286 E287 R288 E304 R318 D329 S330 T331 S332 R333 E340 P349 G350 D351 E352 G353 R371 V372 I373

A374 L375 D378 Q379 R380 E381 S391 P400 F412 S417 Q421 K422 R423 H424 F425 P426 S427 W430 S433 D452 W453 M456 M461 R462 I463 L470 N471 E472 I473 V474 R475 L476 V477 G478 I479 R487 L488 T489 V492 E498 Q502 Q503 D507

D508 V509 D510 T511 E516 K517 Q518 F519 N520 M521 L522 K523 V524 A535 Y541 E544 I545 M546 V550 A551 V552 R553 E554 R555 I556 S557 R558 Y561 I562 P563 E564 E565 E566 S572 E579 THR ILE GLN LEU ILE VAL SER GLU GLY GLY MSE THR ASP ASP

● Molecule 2: V-type sodium ATPase subunit B

Chain D:

81% 15%

GLY SER SER GLY SER GLY MSE ILE LYS | E4 I8 V11 V12 M16 E27 E28 L29 I30 E31 V32 R41 V44 V47 V54 L65 K66 V70 R71 D84 R88 V89 F90 D91 R95 I103 D110 P118 F127 H137 Q145

F150 A162 Q163 R166 L171 D175 D176 F177 A182 D197 M209 A232 E233 Y237 E238 V243 M247 T248 D249 M250 V267 P268 Y276 L277 A288 V298 T299 Q300 I303 L304 P307 E308 L318 E324 I327 L348 S349 R350

L351 K354 G355 T356 H365 Y376 A386 L394 D398 R407 F408 E409 Y412 M436 R444 L449 P455 GLU GLY LYS

● Molecule 2: V-type sodium ATPase subunit B

Chain E:

2%
80% 16%

GLY SER SER GLY SER GLY MSE ILE LYS | E4 Y5 R6 T7 G13 M16 A17 V18 E19 M34 E38 V44 V54 Q55 I56 F57 T60 I63 N64 L65 V70 D91 R95 E106 N112 G113 D122 Y123 P124 D125 E126 F127 I128 Q129 T130 G131

I132 V142 Q145 S151 G152 A168 S173 S174 D175 D176 A182 A183 G185 I186 F193 A214 I219 E220 R221 L229 Y234 M247 T248 D249 M250 T251 N252 Y253 A254 E255 A256 G272 R287 R292 I303 L304 Y321 L329 Q339 P340

L345 L351 G355 T356 K360 T361 R362 E363 D364 N370 K380 E384 V387 V388 S392 A393 D396 Y412 Q415 W431 R444 D447 L454 P455 GLU GLY LYS

● Molecule 2: V-type sodium ATPase subunit B

Chain F:

2%
73% 22%

GLY SER SER GLY SER GLY | M1 I8 V18 E28 R33 M34 I39 R40 V44 L45 E46 V47 V54 S61 G62 I63 N64 L65 F72 L79 I86 D91 G92 L93 G94 R95 P96 K97 E114 P124 D125 E126 Q129 I132 S133 A134

H137 L138 N139 T140 L141 V142 R143 G144 Q145 S151 G152 L155 A161 R166 T169 V170 S173 S174 D175 D176 F177 F181 A182 F193 F194 M195 E196 T201 G202 A203 I204 D205 R206 S207 V208 M209 E220 R221 I222 A231 Y237 I246 M247 T248 D249 L257

R264 R265 E266 Y276 L277 Y278 A288 L294 V298 I301 P302 I303 L304 T305 Y321 E324 G325 I348 S349 R350 L351 K352 D353 K354 G355 R362 E363 D364 T368 M369 L372 F373 L385 A386 L389 G390 E391 L394 S395 D396 I397 I400 Y401

F404 R407 Y412 Q415 T422 L427 D428 L429 G430 W431 E432 L433 M436 R439 T440 K446 D447 D448 D451 K452 Y453 LEU PRO GLY LYS

• Molecule 3: V-type sodium ATPase subunit D

Chain G:

5%

59%   14%   •   24%

GLY SER SER GLY SER SER GLY MSE R2 T8 L12 T23 K27 K30 Q33 D34 E35 R38 Q39 F40 I41 L42 L43 I44 N47 A53 I54 E55 K56 E57 T58 Q59 T60 K63 D64 F65 VAL LEU ALA LYS SER THR VAL GLU GLU ALA F76 L80 L81

A82 L83 PRO ALA E86 N87 V88 SER ILE SER V92 M98 P103 L104 MSE ASN PHE GLN TYR ASP GLU THR LEU ASN GLU THR PRO LEU GLU TYR GLY TYR LEU HIS SER ASN ALA GLU LEU D130 R131 S132 F136 T137 Q138 L139 L140 P141 V149 L155 R165 R166 I182

I185 K188 E191 N192 E193 R194 V197 L200 I201 K202 V203 K204 N205 M206 GLY THR GLU GLU

• Molecule 4: V-type sodium ATPase subunit NtpG (F)

Chain H:

10%

80%   • •   14%

MSE T2 K11 H26 GLY THR T29 E44 Y45 G46 V47 I48 Y49 A55 N56 Q68 L69 T70 P71 I76 P77 I90 V94 I102 LEU SER GLY PRO SER SER GLY GLU ASN LEU TYR PHE GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	127.74Å 128.87Å 231.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.13 – 3.82 46.13 – 3.82	Depositor EDS
% Data completeness (in resolution range)	99.6 (46.13-3.82) 99.5 (46.13-3.82)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.50 (at 3.77Å)	Xtriage
Refinement program	PHENIX 1.12-2829	Depositor
R, R_{free}	0.226 , 0.267 0.226 , 0.267	Depositor DCC
R_{free} test set	1884 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	120.1	Xtriage
Anisotropy	0.552	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 107.5	EDS
L-test for twinning [2]	$< |L| > = 0.44, < L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.048 for k,h,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	25072	wwPDB-VP
Average B, all atoms (Å^2)	148.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.13% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP, ALF, GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.24	0/4373	0.42	0/5921
1	B	0.25	0/4422	0.43	0/5974
1	C	0.25	0/4271	0.42	0/5774
2	D	0.25	0/3423	0.43	0/4628
2	E	0.26	0/3472	0.44	0/4693
2	F	0.26	0/3492	0.46	1/4715 (0.0%)
3	G	0.24	0/1204	0.41	0/1612
4	H	0.25	0/645	0.45	0/887
All	All	0.25	0/25302	0.43	1/34204 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	348	LEU	CA-CB-CG	5.09	127.02	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2   Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4320	0	4062	68	0
1	B	4370	0	4075	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4220	0	3737	58	0
2	D	3375	0	3136	50	0
2	E	3423	0	3194	52	0
2	F	3445	0	3355	83	0
3	G	1207	0	1119	23	0
4	H	639	0	539	6	0
5	A	6	0	8	0	0
6	B	27	0	12	2	0
6	C	27	0	12	3	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	B	5	0	0	3	0
8	C	5	0	0	0	0
9	B	1	0	0	0	0
All	All	25072	0	23249	360	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 360 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:MSE:HG2	2:E:65:LEU:HD21	1.49	0.93
1:C:509:VAL:HG11	1:C:561:TYR:HA	1.53	0.88
2:F:195:MSE:HA	2:F:195:MSE:HE2	1.57	0.87
2:F:385:LEU:HB3	2:F:394:LEU:HD21	1.65	0.79
1:B:214:ARG:NH1	1:B:510:ASP:OD1	2.16	0.78

There are no symmetry-related clashes.

5.3   Torsion angles ⓘ

5.3.1   Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	586/600 (98%)	568 (97%)	18 (3%)	0	100	100
1	B	591/600 (98%)	575 (97%)	16 (3%)	0	100	100
1	C	577/600 (96%)	560 (97%)	17 (3%)	0	100	100
2	D	450/465 (97%)	438 (97%)	12 (3%)	0	100	100
2	E	450/465 (97%)	438 (97%)	12 (3%)	0	100	100
2	F	451/465 (97%)	441 (98%)	10 (2%)	0	100	100
3	G	155/217 (71%)	153 (99%)	2 (1%)	0	100	100
4	H	95/115 (83%)	89 (94%)	6 (6%)	0	100	100
All	All	3355/3527 (95%)	3262 (97%)	93 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	437/487 (90%)	414 (95%)	23 (5%)	22	54
1	B	437/487 (90%)	419 (96%)	18 (4%)	30	59
1	C	394/487 (81%)	366 (93%)	28 (7%)	14	45
2	D	313/372 (84%)	299 (96%)	14 (4%)	27	57
2	E	324/372 (87%)	307 (95%)	17 (5%)	23	54
2	F	349/372 (94%)	326 (93%)	23 (7%)	16	47
3	G	111/188 (59%)	97 (87%)	14 (13%)	4	23
4	H	53/97 (55%)	50 (94%)	3 (6%)	20	52
All	All	2418/2862 (84%)	2278 (94%)	140 (6%)	20	51

5 of 140 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	352	LYS
2	F	396	ASP

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Mol	Chain	Res	Type
3	G	58	THR
1	C	304	GLU
1	C	288	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	HIS
1	A	280	ASN
2	F	129	GLN
3	G	47	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
5	GOL	A	601	-	5,5,5	0.89	0	5,5,5	1.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	ADP	B	601	7	24,29,29	0.97	1 (4%)	29,45,45	1.48	5 (17%)
8	ALF	B	603	-	0,4,4	-	-	-		
8	ALF	C	603	-	0,4,4	-	-	-		
6	ADP	C	601	7	24,29,29	0.97	1 (4%)	29,45,45	1.39	4 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	601	-	-	0/4/4/4	-
6	ADP	C	601	7	-	3/12/32/32	0/3/3/3
6	ADP	B	601	7	-	3/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	601	ADP	C5-C4	2.53	1.47	1.40
6	C	601	ADP	C5-C4	2.51	1.47	1.40

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	601	ADP	C3'-C2'-C1'	3.20	105.79	100.98
6	B	601	ADP	N3-C2-N1	-3.13	123.79	128.68
6	C	601	ADP	N3-C2-N1	-3.09	123.84	128.68
6	B	601	ADP	PA-O3A-PB	-3.07	122.31	132.83
6	C	601	ADP	PA-O3A-PB	-3.04	122.41	132.83

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	601	ADP	PA-O3A-PB-O2B
6	C	601	ADP	PA-O3A-PB-O2B
6	B	601	ADP	PA-O3A-PB-O1B
6	C	601	ADP	PA-O3A-PB-O1B
6	B	601	ADP	PA-O3A-PB-O3B

There are no ring outliers.
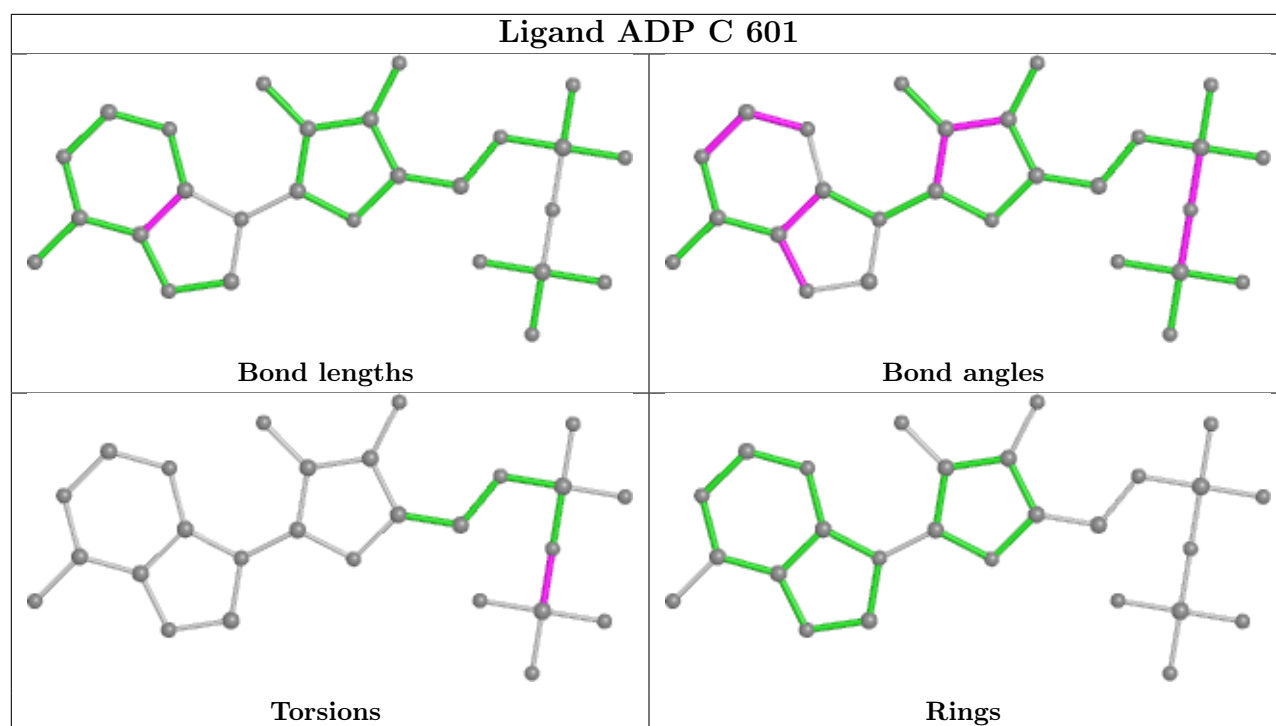
3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	601	ADP	2	0
8	B	603	ALF	3	0
6	C	601	ADP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ADP B 601

Bond lengths

Bond angles

Torsions

Rings

Ligand ALF B 603

Bond lengths

Bond angles

Torsions

Rings

Ligand ALF C 603

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP C 601

Bond lengths

Bond angles

Torsions

Rings
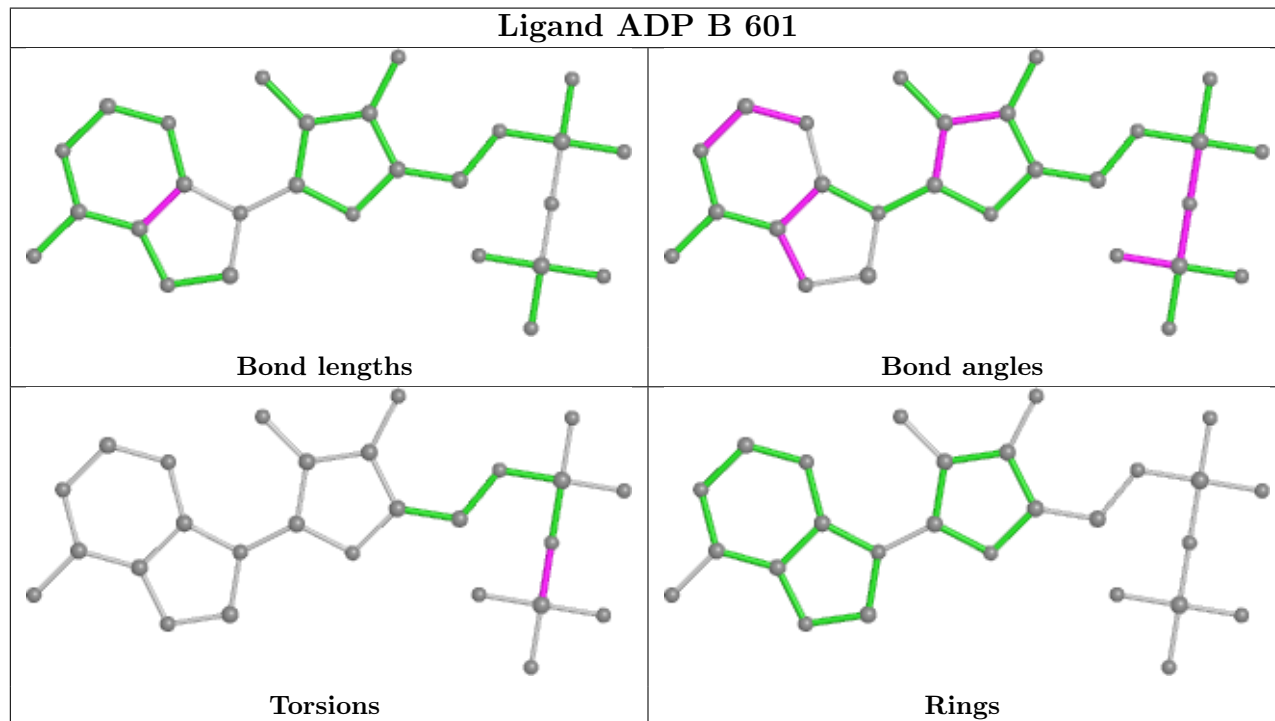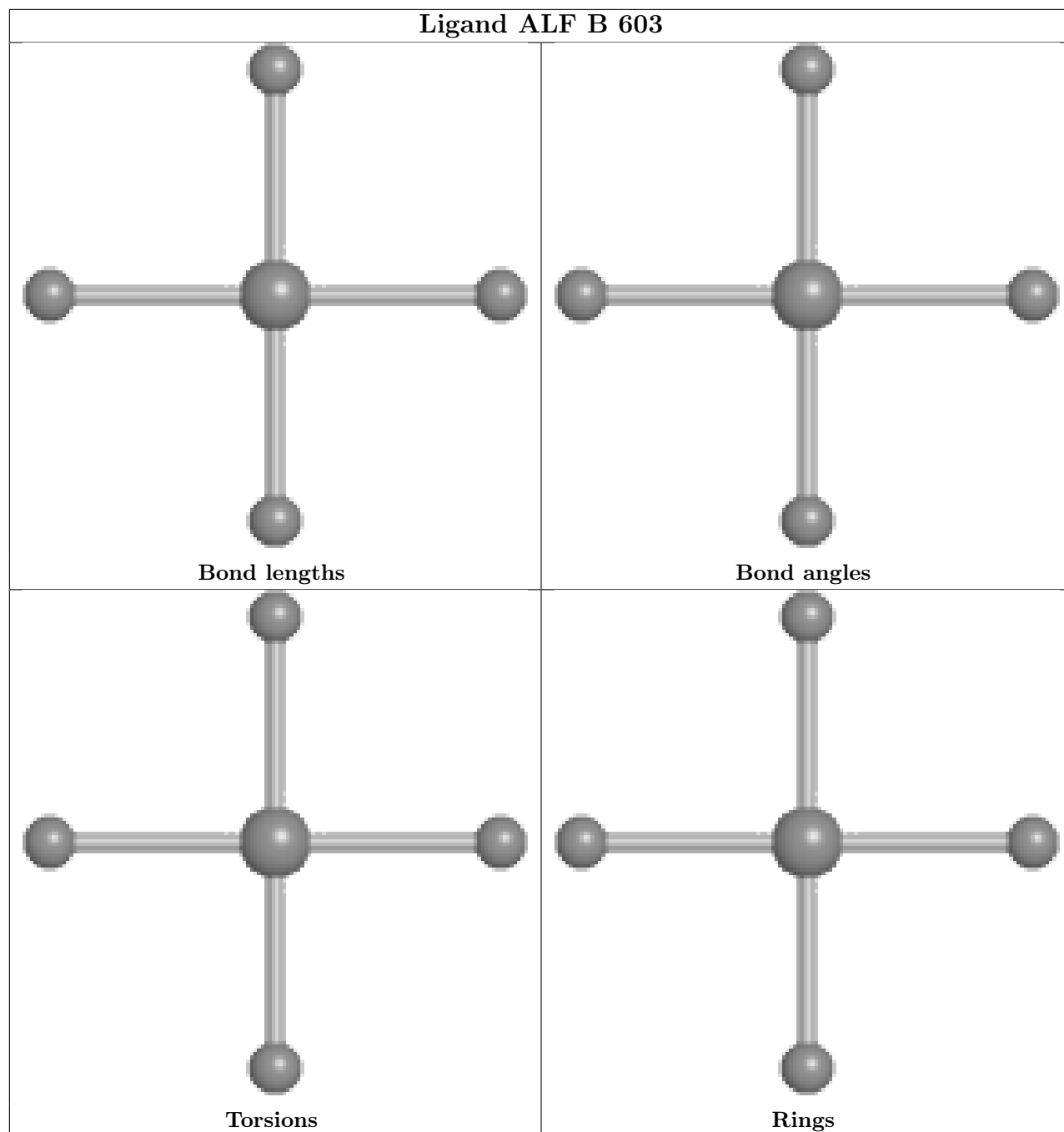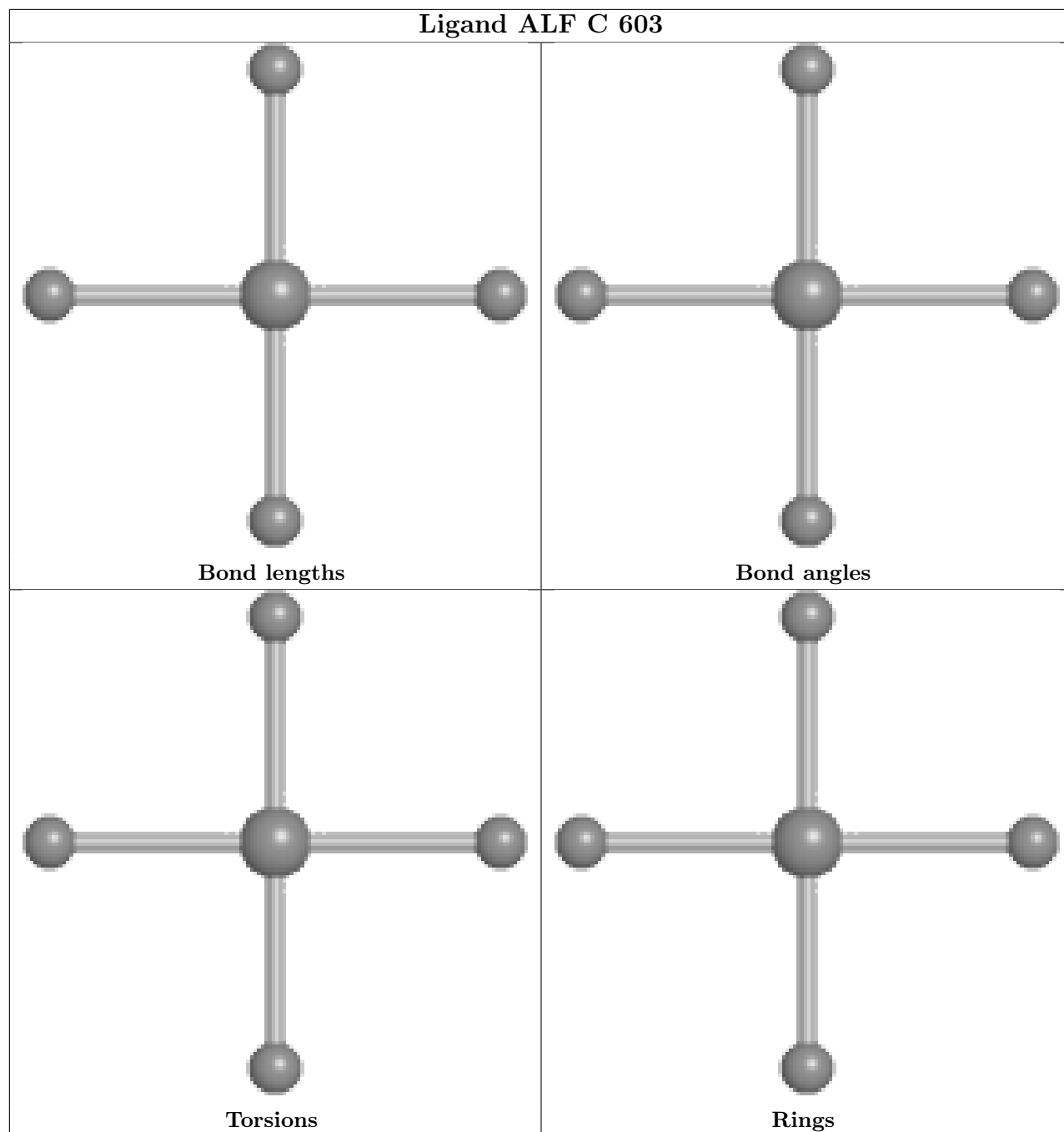
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6   Fit of model and data ⓘ

6.1   Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	565/600 (94%)	0.03	20 (3%)	44	35	83, 140, 192, 219	0
1	B	570/600 (95%)	0.10	18 (3%)	47	38	82, 142, 215, 264	0
1	C	556/600 (92%)	0.10	23 (4%)	37	31	99, 150, 229, 266	0
2	D	438/465 (94%)	-0.10	2 (0%)	91	86	84, 138, 201, 228	0
2	E	438/465 (94%)	-0.15	7 (1%)	72	64	70, 122, 169, 218	0
2	F	438/465 (94%)	-0.01	10 (2%)	60	52	87, 151, 218, 240	0
3	G	157/217 (72%)	0.29	10 (6%)	19	14	97, 164, 282, 304	0
4	H	98/115 (85%)	0.62	11 (11%)	5	5	108, 221, 271, 277	0
All	All	3260/3527 (92%)	0.04	101 (3%)	49	39	70, 142, 221, 304	0

The worst 5 of 101 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	124	ILE	5.9
2	F	364	ASP	5.3
1	B	174	CYS	4.7
1	B	125	GLU	4.5
1	C	174	CYS	4.5

6.2   Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3   Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GOL	A	601	6/6	0.80	0.57	101,108,117,121	0
6	ADP	B	601	27/27	0.91	0.30	78,107,126,134	0
6	ADP	C	601	27/27	0.91	0.32	95,127,151,162	0
7	MG	C	602	1/1	0.91	0.70	144,144,144,144	0
8	ALF	C	603	5/5	0.91	0.52	101,110,129,135	0
8	ALF	B	603	5/5	0.93	0.41	111,112,155,160	0
7	MG	B	602	1/1	0.98	0.47	76,76,76,76	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.
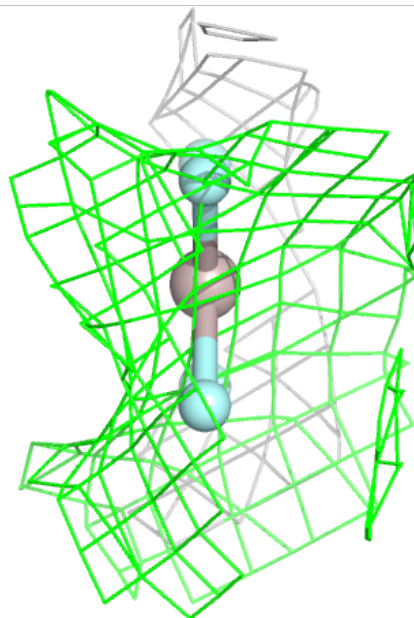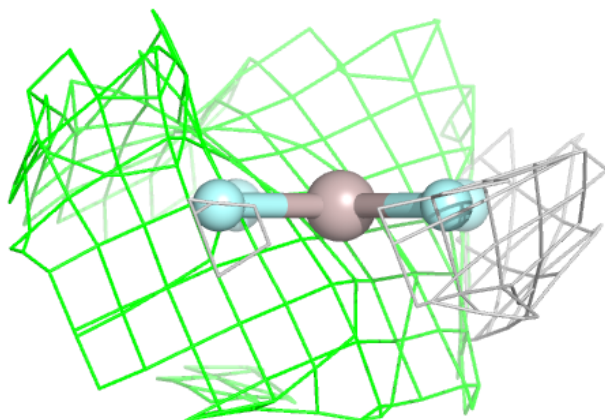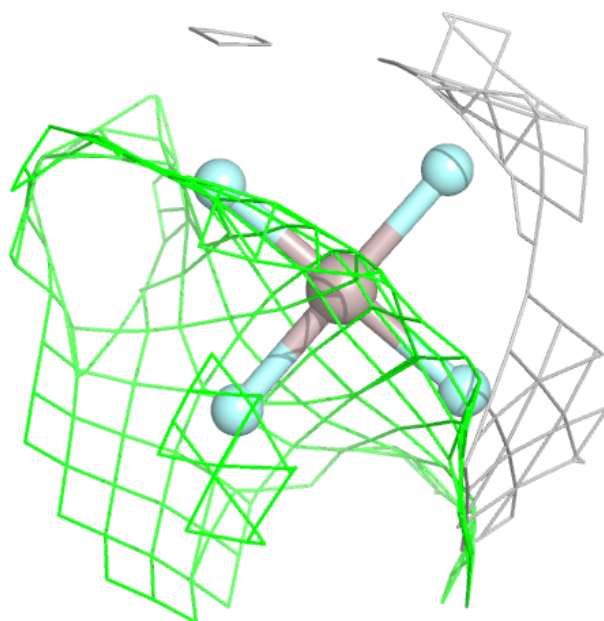
Electron density around ADP B 601:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
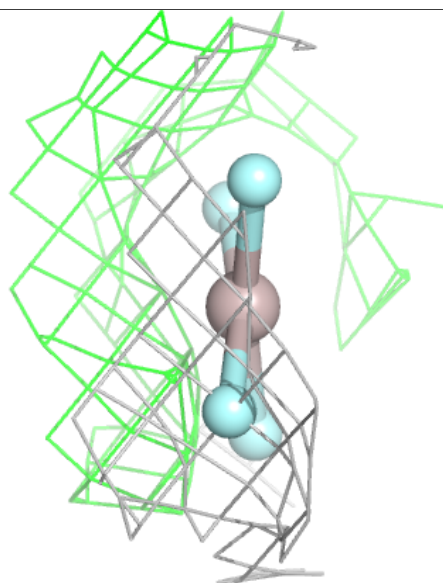$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative) and green (positive)
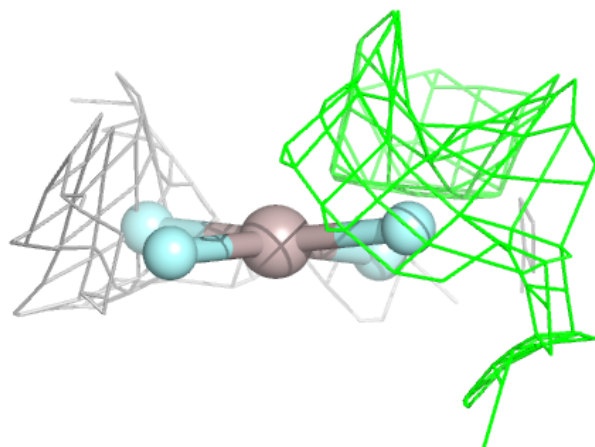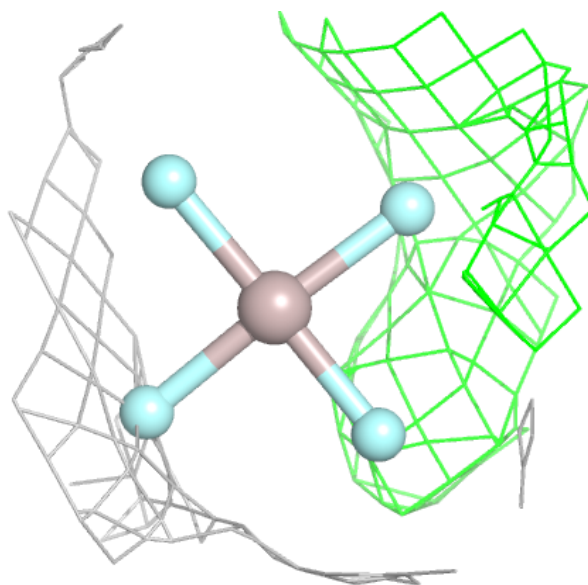
Electron density around ADP C 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
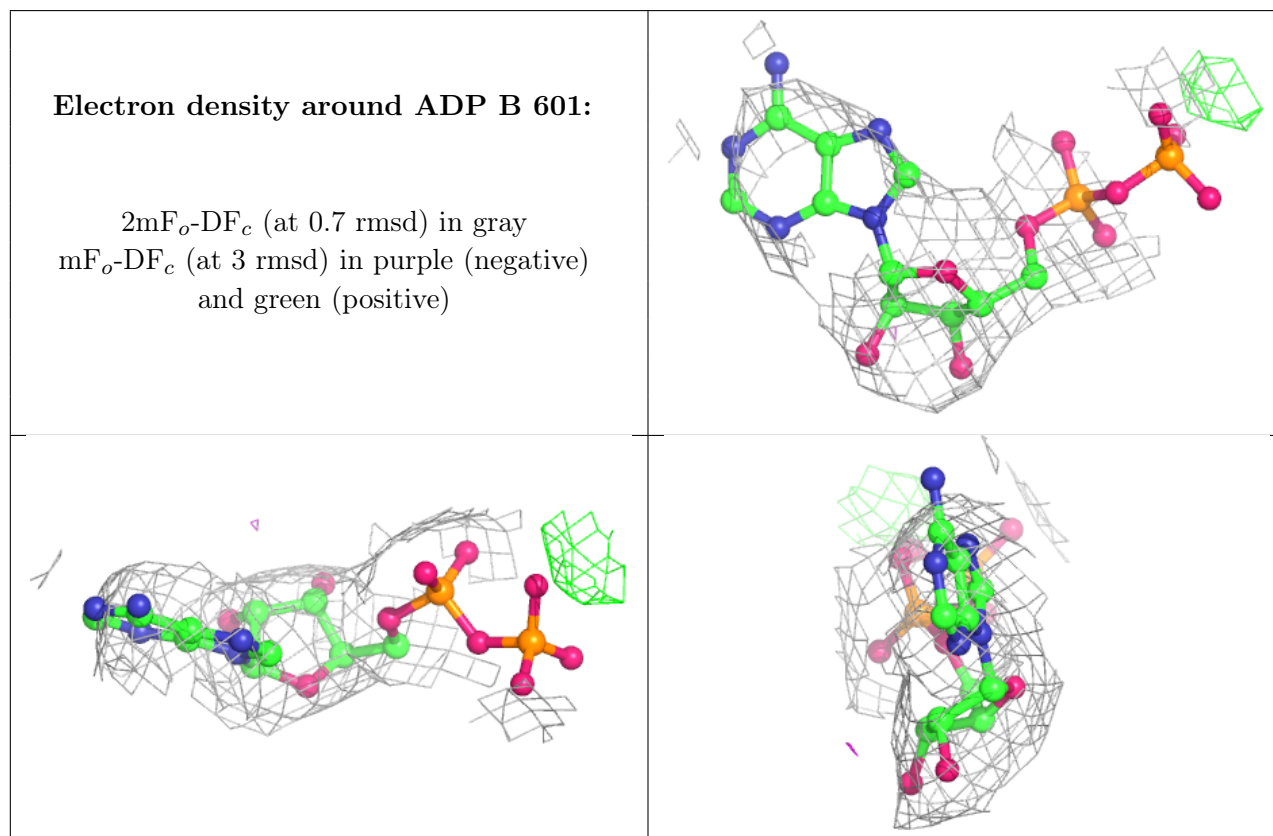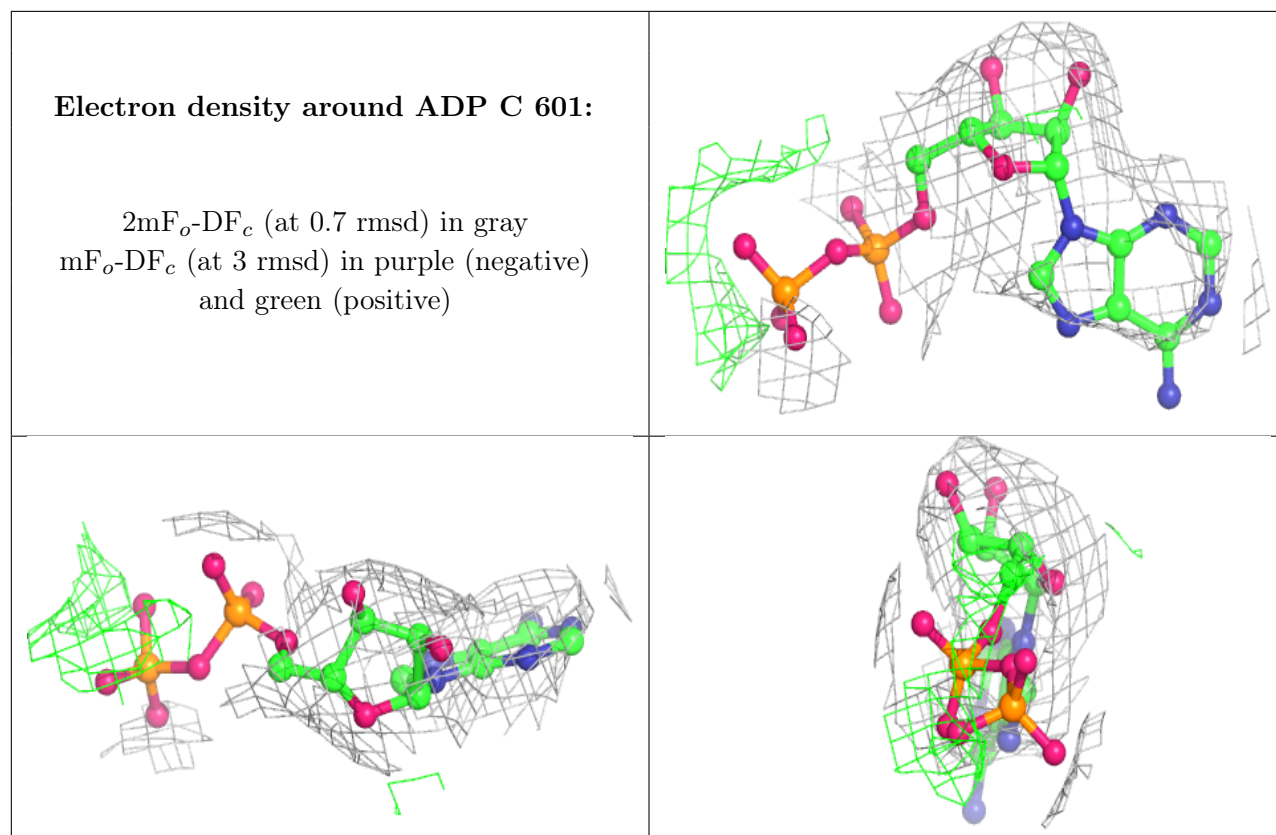
Electron density around MG C 602:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
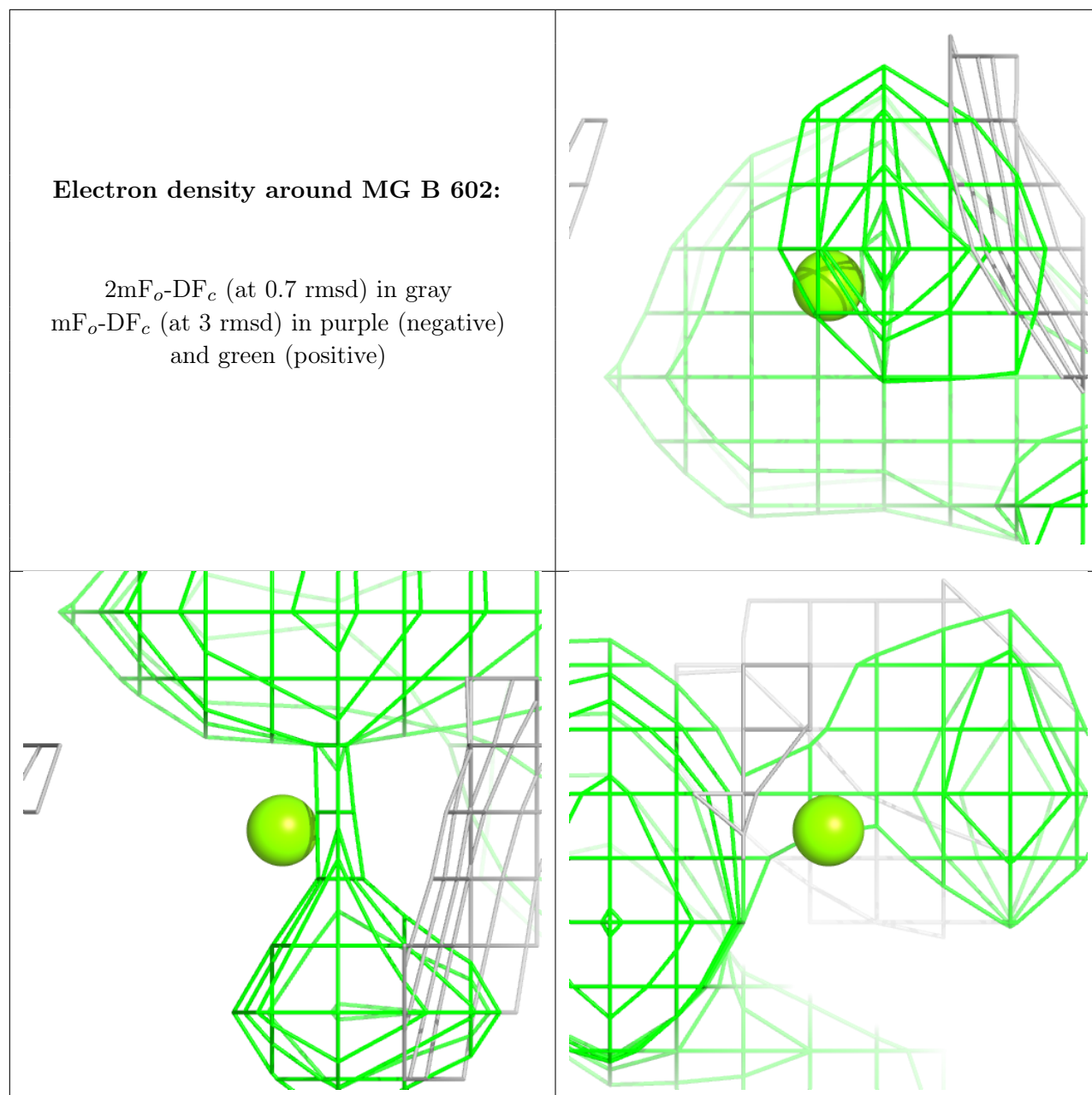and green (positive)
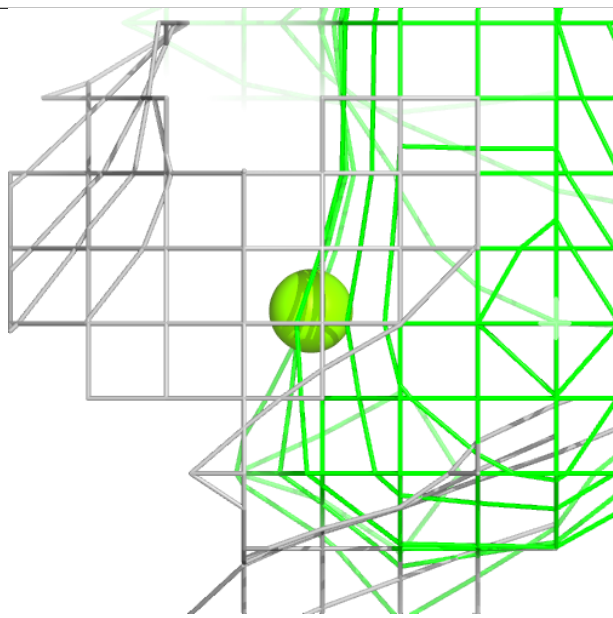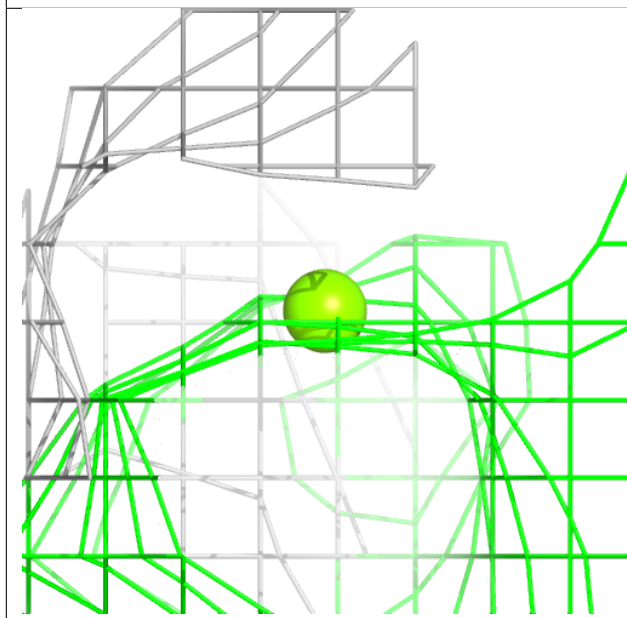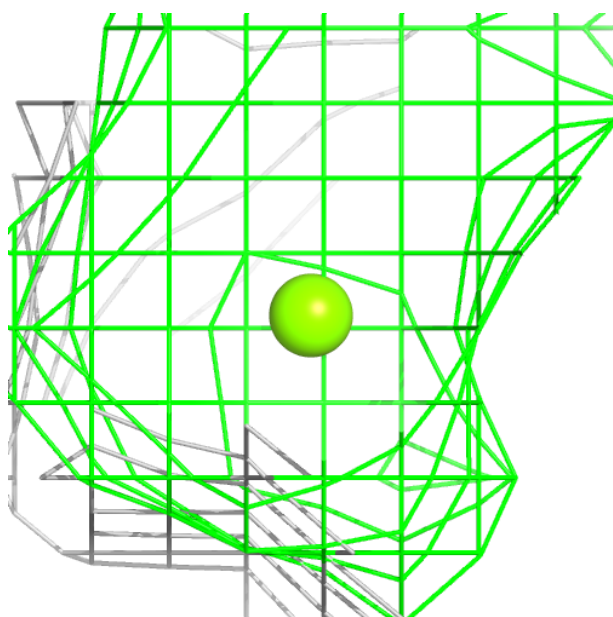
Electron density around ALF C 603:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around ALF B 603:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around MG B 602:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

6.5　Other polymers ⓘ

There are no such residues in this entry.